A Route to Highly Functionalized stereospecific trans-Aminated Aurones from 3-bromoflavones with aniline and N-phenyl urea via a Domino Aza Michael ring opening and cyclization reactions

Iram Parveen and Naseem Ahmed*
Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee 247 667, India
*Corresponding author. Fax and Tel.: +91 1332 285745
*E-mail: nasmfcy@iitr.ac.in

1) $^1$H and $^{13}$C NMR data for the compounds prepared
2) Crystal data

2-39
39-40
Fig. S1: $^1$H and $^{13}$C spectra of 2a in CDCl$_3$
Fig. S2: $^1$H and $^{13}$C spectra of 2b in CDCl$_3$
Fig. S3: $^1$H and $^{13}$C spectra of 2c in CDCl$_3$
**Fig. S4:** $^1$H and $^{13}$C spectra of 2d in CDCl$_3$
Fig. S5: $^1$H and $^{13}$C spectra of 2e in CDCl$_3$
Fig. S6: $^1$H and $^{13}$C spectra of 2f in CDCl$_3$
Fig. S7: $^1$H and $^{13}$C spectra of 2g in CDCl$_3$
Fig. S8: $^1$H and $^{13}$C spectra of 2h in CDCl$_3$
Fig. S9: $^1$H and $^{13}$C spectra of 2i in CDCl$_3$
Fig. S10: $^1$H and $^{13}$C spectra of 2j in CDCl$_3$
Fig. S11: $^1$H and $^{13}$C spectra of 2\textit{k} in CDCl$_3$
Fig. S12: $^1$H and $^{13}$C spectra of 2l in CDCl$_3$
Fig. S13: $^1$H and $^{13}$C spectra of 2m in CDCl$_3$
Fig. S14: $^1$H and $^{13}$C spectra of 2n in CDCl$_3$
Fig. S15: $^1$H and $^{13}$C spectra of 2o in CDCl$_3$
Fig. S16: $^1$H and $^{13}$C spectra of 2p in CDCl$_3$
Fig.S17: $^1$H and $^{13}$C spectra of 2q in CDCl$_3$
Fig. S18: $^1$H and $^{13}$C spectra of 2r in CDCl$_3$
Fig.S19: $^1$H and $^{13}$C spectra of 2s in CDCl$_3$
Fig. S20: $^1$H and $^{13}$C spectra of 2t in CDCl$_3$.
Fig. S21: $^1$H and $^{13}$C spectra of 2u in CDCl$_3$
Fig.S22: $^1$H and $^{13}$C spectra of 2v in CDCl$_3$
Fig. S23: $^1$H and $^{13}$C spectra of 2w in CDCl$_3$
Fig. S24: $^1$H and $^{13}$C spectra of 2x in CDCl$_3$
Fig.S24: $^1$H and $^{13}$C spectra of 2y in CDCl$_3$
Fig. S25: $^1$H and $^{13}$C spectra of 4a in CDCl$_3$
Fig. S26: $^1$H and $^{13}$C spectra of 4b in CDCl$_3$
Fig. S27: $^1$H and $^{13}$C spectra of 4c in CDCl$_3$
Fig. S28: $^1$H and $^{13}$C spectra of 4d in CDCl$_3$
Fig. S29: $^1$H and $^{13}$C spectra of 4e in CDCl$_3$
Fig.S30: $^1$H and $^{13}$C spectra of 4f in CDCl$_3$
Fig. S31: $^1$H and $^{13}$C spectra of 4g in CDCl$_3$
Fig. S32: $^1$H and $^{13}$C spectra of 4h in CDCl$_3$
Fig. S3: $^1$H and $^{13}$C spectra of 5a in CDCl$_3$
Fig. S34: $^1$H and $^{13}$C spectra of 5b in CDCl$_3$
Fig.S3: $^1$H and $^{13}$C spectra of 5c in CDCl$_3$
Fig. S36: $^1$H and $^{13}$C spectra of 5d in CDCl$_3$
X-Ray crystallographic information of products 4b:

Single crystal of product 4b was obtained through slow evaporation (at room temperature) of a solution in dichloromethane-methanol. Single crystal data of products 3a were collected on X-ray diffractometer using graphite monochromatedMoKα radiation (λ = 0.7106 Å) at 293 K. Suitable size of crystals reported here were mounted on nylon CryoLoop. In the reduction of data Lorentz and polarization corrections, empirical absorption corrections were applied. Crystal structures were solved by direct method. Structure solution, refinement and data output were carried out with the SHELXTL program.\(^2\)\(^3\) Non-hydrogen atoms were refined anisotropically. Refinements were carried out with a full matrix least squares method against F2 using the SHELXTL program. Structure was examined using the ADDSYM sub-routine of PLATON 4 to 14 assures that no additional symmetry could be applied to the models.

REFERENCES

**ORTEP:** Plot of Compound 4b
Table S2: Important crystal data of compound 4b

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Empirical formula</td>
<td>C19 H12 N2 O5</td>
</tr>
<tr>
<td>Formula weight</td>
<td>348.31</td>
</tr>
<tr>
<td>Temperature</td>
<td>293 K</td>
</tr>
<tr>
<td>Wavelength</td>
<td>0.71073</td>
</tr>
<tr>
<td>Space group</td>
<td>P -1 P -1</td>
</tr>
<tr>
<td>Unit cell dimensions</td>
<td>a=9.6749(4) Å , α = 77.974°</td>
</tr>
<tr>
<td></td>
<td>b= 12.6311(6) Å , β = 84.075°</td>
</tr>
<tr>
<td></td>
<td>c= 13.4296(6) Å , γ = 85.172°</td>
</tr>
<tr>
<td>Volume</td>
<td>1593.25(12)</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
</tr>
<tr>
<td>Density (calculated)</td>
<td>1.452g/cm³</td>
</tr>
<tr>
<td>Absorption coefficient (μ)</td>
<td>0.107 (mm⁻¹)</td>
</tr>
<tr>
<td>F(000)</td>
<td>392.0</td>
</tr>
<tr>
<td>h,k,l max</td>
<td>12,16,17</td>
</tr>
<tr>
<td>Nref</td>
<td>7943</td>
</tr>
<tr>
<td>Data completeness</td>
<td>0.987</td>
</tr>
<tr>
<td>Absorption correction</td>
<td>MULTI-SCAN</td>
</tr>
<tr>
<td>Theta max</td>
<td>28.357</td>
</tr>
<tr>
<td>Refinement method</td>
<td>Full-matrix least-squares on F²</td>
</tr>
<tr>
<td>R(reflections)</td>
<td>0.0568( 4509)</td>
</tr>
<tr>
<td>wR2(reflections)</td>
<td>0.2321( 7840)</td>
</tr>
</tbody>
</table>

The crystal data of product 4b has been deposited at Cambridge Crystallographic Data Centre. The CCDC reference number is 1577307.